Treatment of Nonuniform Temperature Distribution by Subgroup Method

Qingming He,[1, 2] Liangzhi Cao,[1] Hongchun Wu,[1] Benoit Forget,[2]* Kord Smith,[2]

[1]*Xi'an Jiaotong University, No.28, Xianning West Road, Xi'an, Shaanxi, 710049, China*
[2]*Massachusetts Institute of Technology, 77 Massachusetts Avenue Cambridge, MA 02139, United States*
**bforget@mit.edu*

INTRODUCTION

The subgroup method divides an energy group into several subgroups according to the magnitude of the cross section. The subgroup fixed source equation is formulated on the energy range of a subgroup, the ratio of which to the energy range of an energy group is defined as subgroup probability. Typically the physical probability table or the mathematical probability table is applied[1]. However, both of the tables are not guaranteed to share the same set of subgroup probabilities for a resonant nuclide at different temperatures. This means that the subgroup fixed source equation cannot be formulated and the subgroup method will not work when the temperature distribution is nonuniform.

To overcome this defect, the subgroup method based on partial cross section fit scheme (PXSFS) and the simplified partial cross section fit scheme (SPXSFS) are proposed. These methods fit the cross sections at different temperatures as partial cross sections to share a same set of subgroup probabilities. The new methods is compared to the conventional subgroup method (CSM) based on physical probability table[2] and the preexisting methods: the correlation model (CM)[3, 4], the subgroup level adjustment scheme (SLAS)[5] and the number density adjustment scheme (NDAS)[6]. The numerical results show that the new methods can better predict the spatial dependent reaction rate than preexisting methods. Within these two methods, the simplified scheme consumes less time.

THEORY

Conventional Subgroup Method

There are different implementations of subgroup method. The subgroup method based on intermediate resonance approximation and homogeneous physical probability table will be discussed in this paper. The subgroup cross sections and subgroup probabilities are obtained by preserving cross sections over a range of background cross sections:

$$\begin{aligned}\sigma_{x,g}(\sigma_\mathrm{b}) &= \frac{\int_{\Delta u_g}\sigma_x(u)\phi(u)\,\mathrm{d}u}{\int_{\Delta u_g}\phi(u)\,\mathrm{d}u}\\ &= \frac{\sum_i\int_{\Delta u_i}\sigma_x(u)\phi(u)\,\mathrm{d}u}{\sum_i\int_{\Delta u_i}\phi(u)\,\mathrm{d}u}\\ &= \frac{\sum_i\sigma_{x,i}\phi_i}{\sum_i\phi_i}\\ &= \frac{\sum_i\sigma_{x,i}\frac{p_i\sigma_\mathrm{b}}{\sigma_{\mathrm{inter},i}+\sigma_\mathrm{b}}}{\sum_i\frac{p_i\sigma_\mathrm{b}}{\sigma_{\mathrm{inter},i}+\sigma_\mathrm{b}}}\end{aligned} \tag{1}$$

where subscript x is reaction type; i is subgroup index; σ_b is background cross section; $\sigma_{x,i}$ is subgroup cross section; ϕ_i is subgroup flux; p_i is subgroup probability; $\sigma_{\mathrm{inter},i}$ is intermediate subgroup cross section defined as $\sigma_{\mathrm{inter},i} = \sigma_{\mathrm{a},i} + \sigma_{\mathrm{sr},i}$.

Firstly, the intermediate subgroup cross sections and subgroup probabilities are obtained by simultaneous fitting. Then the partial subgroup cross sections, including total subgroup cross sections, absorption subgroup cross sections, scatter subgroup cross sections and neutron production subgroup cross sections, are obtained by fitting with fixed subgroup probabilities.

The subgroup fixed source equation based on intermediate resonance approximation is formulated as:

$$\begin{aligned}&\mathbf{\Omega}\cdot\nabla\psi_i(\mathbf{r},\mathbf{\Omega}) + \Sigma_{\mathrm{t},i}(\mathbf{r})\psi_i(\mathbf{r},\mathbf{\Omega})\\ &\qquad = \frac{1}{4\pi}\left[p_i\Delta u_g\lambda\Sigma_\mathrm{p}(\mathbf{r}) + (1-\lambda)\Sigma_{\mathrm{s},i}(\mathbf{r})\phi_i(\mathbf{r})\right]\end{aligned} \tag{2}$$

where $\Sigma_{\mathrm{t},i}$ is macroscopic total subgroup cross section; $\Sigma_{\mathrm{s},i}$ is macroscopic scatter subgroup cross section; λ is Goldstein-Cohen factor; Σ_p is potential scatter cross section.

Once equation (2) is solved, the effective self-shielded cross section can be obtained by:

$$\sigma_{x,g}(\mathbf{r}) = \frac{\sum_i\sigma_{x,i}\phi_i(\mathbf{r})}{\sum_i\phi_i(\mathbf{r})} \tag{3}$$

For problems with nonuniform temperature distribution, the p_i and the corresponding energy range will be different at different temperatures. Therefore equation (2) cannot be formulated. The preexisting methods and the new method are trying to unify the subgroup probabilities at different temperatures.

Correlation Model

The basic idea of the correlation model[3, 4] is to find the overlap energy range of subgroups at different temperatures after obtaining probability tables at different temperatures respectively. For a case with two temperatures, a new subgroup probability $p_{T_1 i,T_2 j}$ is defined to denotes the ratio of overlap energy range of subgroup i at temperature T_1 and subgroup j at temperature T_2 to the energy range of an energy group. For a case with more temperatures, the overlap energy range at all temperatures should be found. Then the probability table is obtained based on the newly defined subgroup probabilities. Accordingly, the subgroup fixed source equations are formulated on the overlap energy ranges.

The disadvantage of this method is that the number of subgroups will increase with increasing number of temperatures. Generally, the number of subgroups can be calculated

as:

$$N = \sum_l N_{T_l} - N_T + 1 \tag{4}$$

where N_{T_l} is number of subgroup at temperature T_l and N_T is number of temperatures.

Subgroup Level Adjustment Scheme

The subgroup level adjustment scheme[5] forces the subgroup probabilities at different temperatures to be the same. Then the subgroup level (subgroup cross section) is adjusted as:

$$\sigma_i'(T) = \frac{p_i(T)}{p_i(T_{\text{ave}})}\sigma_i(T) \tag{5}$$

where T_{ave} is average temperature.

If the average temperature is 975 K, the subgroup cross sections are adjusted by equation (5). Then the absorption cross sections at different dilutions and different temperatures of ^{238}U are recovered by probability table according to equation (1). It is found that the absorption cross sections at all dilutions except infinite dilution will not be preserved after subgroup level adjustment (Figure 1).

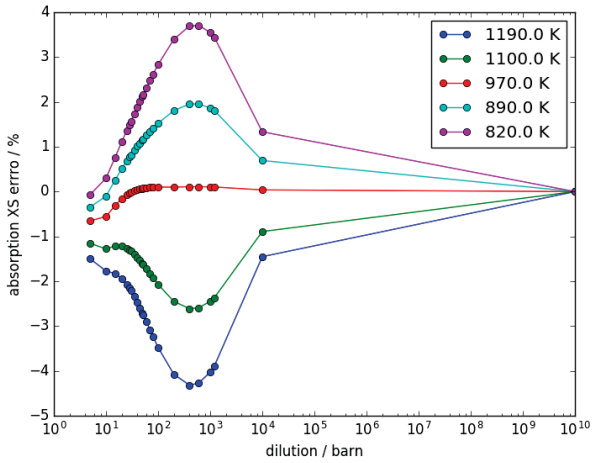

Fig. 1. ^{238}U absorption cross section errors at different dilutions and different temperatures after adjustment of 27th group (4.0 eV 9.877 eV)

Number Density Adjustment Scheme

The macroscopic subgroup cross section used in the subgroup fixed source equation is written as:

$$\begin{aligned}\Sigma_{i,k}(T) &= N_k\sigma_{i,k}(T)\\ &= N_k\frac{\sigma_{i,k}(T)}{\sigma_{i,k}(T_{\text{ave}})}\sigma_{i,k}(T_{\text{ave}})\\ &= N_k f_{i,k}\sigma_{i,k}(T_{\text{ave}})\end{aligned} \tag{6}$$

where $f_{i,k}$ is the number density adjustment factor. In practical, the subgroup cross sections and subgroup probabilities at average temperature is used and the adjustment factor is applied to the number density.

The adjustment factor is calculated as:

$$f_{i,k}(T) = \frac{\sigma_{i,k}(T)}{\sigma_{i,k}(T_{\text{ave}})} \approx \frac{\sigma_k(T,\sigma_{\text{b}})}{\sigma_k(T_{\text{ave}},\sigma_{\text{b}})} \tag{7}$$

The procedure for the adjustment factor calculation is as follows:

1. Perform self-shielding calculation by conventional subgroup method with average temperature assumption and obtain the self-shielded absorption cross sections for each region;
2. Obtain the background cross sections for each region by interpolation in the resonance cross section table at T_{ave};
3. Obtain the self-shielded cross section at T by interpolation with known background cross section;
4. Calculate the adjustment factor for each region according to equation (7).

Partial Cross Section Fit Scheme

Firstly let's revisit the assumption made in the ISDDM[7]. The ^{238}U absorption reaction rate will increase in the center while decrease in the peripheral when nonuniform temperature distribution is considered. However, the flux will not change much for case with nonuniform temperature distribution.

In light of this, a new kind of partial cross section is defined as:

$$\begin{aligned}\sigma'_{x,g}(\sigma_{\text{b}},T) &= \frac{\int_{\Delta u_g}\sigma_x(u,T)\phi(u,T_{\text{eff}})\,\text{d}u}{\int_{\Delta u_g}\phi(u,T_{\text{eff}})\,\text{d}u}\\ &= \frac{\sum_i\int_{\Delta u_i}\sigma_x(u,T)\phi(u,T_{\text{eff}})\,\text{d}u}{\sum_i\int_{\Delta u_i}\phi(u,T_{\text{eff}})\,\text{d}u}\\ &= \frac{\sum_i\sigma_{x,i}(T)\frac{p_i\sigma_{\text{b}}}{\sigma_{\text{inter},i}(T_{\text{eff}})+\sigma_{\text{b}}}}{\sum_i\frac{p_i\sigma_{\text{b}}}{\sigma_{\text{inter},i}(T_{\text{eff}})+\sigma_{\text{b}}}}\end{aligned} \tag{8}$$

where $\sigma'_{x,g}(\sigma_{\text{b}},T)$ is the partial cross section of x reaction type at background σ_{b} and temperature T of group g; $\phi(u,T_{\text{eff}})$ is solution of neutron slowing-down problem at temperature T_{eff}; T_{eff} is the effective temperature defined to preserve absorption reaction rate; $\sigma_{\text{inter},i}(T_{\text{eff}})$ is the intermediate subgroup cross section at effective temperature; $\sigma_{x,i}(T)$ is the partial subgroup cross section at temperature T.

Based on equation (8), the new calculation procedure is as follows:

1. Perform self-shielding calculation by conventional subgroup method with average temperature assumption and obtain the absorption reaction rate of the fuel region as $R_{\text{a}} = \int\sum_i\phi_i(\mathbf{r})\sigma_{\text{a},i}\,\text{d}\mathbf{r}$;
2. Guess an effective temperature and solve the neutron slowing-down equation over a range dilutions at the temperature. Obtain the multi-group cross section $\sigma_{x,g}(\sigma_{\text{b}},T_{\text{eff}})$ and continuous-energy flux $\phi(u,T_{\text{eff}})$. Use the flux to condense continuous-energy cross sections at all other temperatures and obtain $\sigma_{x,g}(\sigma_{\text{b}},T)$;

3. Fit intermediate subgroup cross sections and subgroup probabilities at effective temperature simultaneously. Then fit total subgroup cross section, absorption subgroup cross section, scatter subgroup cross section and neutron product subgroup cross section at effective temperature and other temperatures as partial subgroup cross sections;

4. Since the subgroup probabilities are shared among different temperatures, the subgroup fixed source equation can be formulated normally. Solve the equation and obtain subgroup flux $\phi_i(\mathbf{r})$. Calculate the spatial dependent self-shielded cross section as $\sigma_{x,g}(\mathbf{r}) = \frac{\sum_i \sigma_{x,i}(T)\phi_i(\mathbf{r})}{\sum_i \phi_i(\mathbf{r})}$. Obtain the absorption reaction rate $R'_{\mathrm{a}} = \int \sum_i \phi_i(\mathbf{r})\sigma_{\mathrm{a},i}(T)\,\mathrm{d}\mathbf{r}$;

5. Iterate from step 2 to step 4 until the effective temperature is found to preserve the reaction rate obtained in the first step.

As the above procedure required searching effective temperature and thus is time consuming, a simplified partial cross section fit scheme is proposed. It is assumed that the differences between spatial dependent cross section shape at effective temperature and that at average temperature are small. The simplified procedure is as follows:

1. Perform self-shielding calculation by conventional subgroup method with average temperature assumption. Obtain spatial dependent self-shielded cross sections $\sigma_{x,g,\mathrm{conv}}(T_{\mathrm{ave}}, \mathbf{r})$ and pin-averaged self-shielded cross section $\sigma_{x,g,\mathrm{conv}}(T_{\mathrm{ave}})$;

2. Perform step 2 to step 4 described above with average temperature. Obtain $\sigma_{x,g,\mathrm{partial}}(T_{\mathrm{ave}}, \mathbf{r})$ and $\sigma_{x,g,\mathrm{parital}}(T_{\mathrm{ave}})$;

3. Correct the self-shielded cross section as $\sigma_{x,g}(\mathbf{r}) = \sigma_{x,g,\mathrm{partial}}(T_{\mathrm{ave}}, \mathbf{r})\frac{\sigma_{x,g,\mathrm{conv}}(T_{\mathrm{ave}})}{\sigma_{x,g,\mathrm{parital}}(T_{\mathrm{ave}})}$

RESULTS AND ANALYSIS

The Monte Carlo code OpenMC is used to generate multi-group library based on JEFF-3.2. The WIMS 69 energy group structure is adopted. The subgroup fixed source equation is solved by OpenMOC and the neutron slowing-down equation is solved by an in-house code to generate resonance cross section tables on line.

A simple pin cell problem is tested to compare the new methods, conventional subgroup method with uniform temperature distribution and preexisting methods. As shown in Figure 2, The pin cell is composed of ten equal-volume fuel regions and a moderator region. The composition of the fuel is ^{238}U with the number density to be 0.0221546 atoms/barn-cm and the composition of the moderator is ^{1}H with the number density to be 0.0662188 atoms/barn-cm. The radius and the pitch is 0.41 cm and 1.26 cm respectively. The temperatures of two cases for each region are given in Table I.

The reference results are obtained by OpenMC. All the results below are given in resonance energy range (4.0 eV 9118.0 eV) as a whole. "Absorption error" means the error of

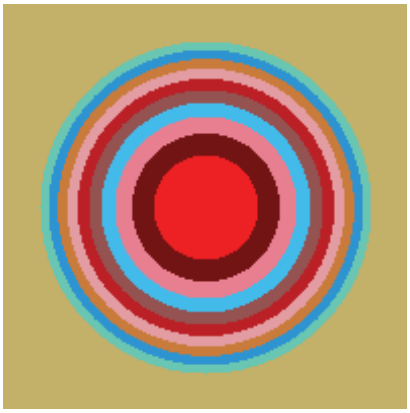

Fig. 2. Configuration of the pin cell problem

Region	Case 1	Case 2
Fuel 1	1190	820
Fuel 2	1140	860
Fuel 3	1100	890
Fuel 4	1060	930
Fuel 5	1010	970
Fuel 6	970	1010
Fuel 7	930	1060
Fuel 8	890	1100
Fuel 9	860	1140
Fuel 10	820	1190
Fuel average	975	1010
Moderator	600	600

TABLE I. Temperatures of two cases for each region

absorption reaction rate for fuel regions as a whole. "RMS" means the root mean square error of absorption errors of all fuel regions. "AVE" means the average error of absorption errors of all fuel regions. For case 1, Figure 3 shows the spatial dependent absorption reaction error for resonance energy range (4.0 eV 9118.0 eV) as a whole. It can be observed that CSM, SLAS and NDAS will underestimate the reaction rate in the center and overestimate in the peripheral. CM, PXSFS and SPXSFS predict spatial dependent reaction rate better. Table II gives the summation of errors. SPXSFS performs best in terms of RMS, which indicates the precision of reaction rate distribution. It is interesting that the SPXSFS outperforms PXSFS in this case. The reason is not fully understood yet and further research is needed. For case 2, Figure 4 shows that CSM, SLAS and NDAS will overestimate the reaction rate in the center and overestimate in the peripheral. CM, PXSFS and SPXSFS predict reaction rate better. Table III summarizes the errors of the methods, within which the PXSFS and SPXSFS perform best in terms of RMS.

CONCLUSIONS

The subgroup method based on partial cross section fit scheme and simplified partial cross section fit scheme are proposed and compared to preexisting methods. The numer-

ical results show that the new methods performs better than other methods in predicting reaction rate distribution with nonuniform temperature distribution. Comparing these two new methods, the simplified scheme requires less computation time.

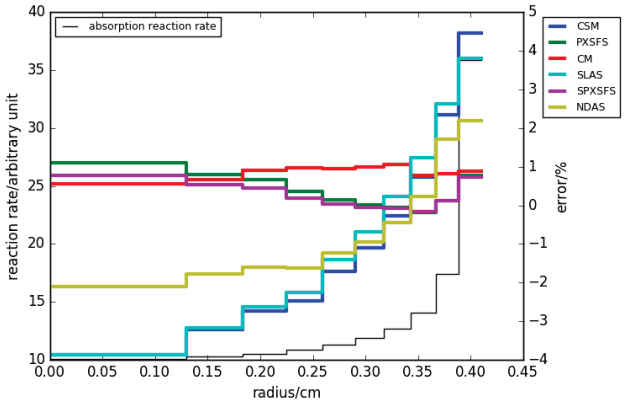

Fig. 3. Spatial dependent percent absorption reaction rate errors of case 1

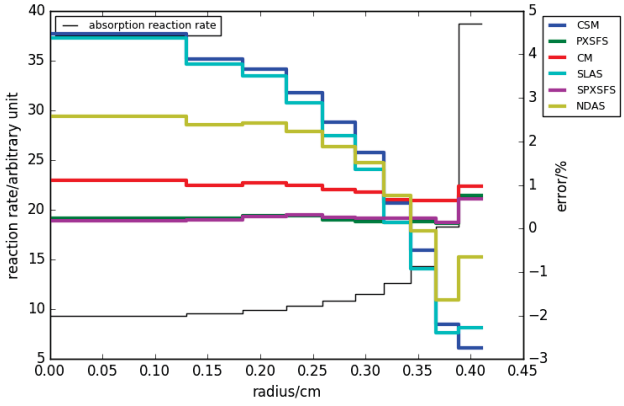

Fig. 4. Spatial dependent percent absorption reaction rate errors of case 2

Method	Absorption error/%	RMS/%	AVE/%
CSM	0.33	2.62	-0.78
SLAS	0.37	2.49	-0.61
NDAS	0.05	1.52	-0.55
CM	0.87	0.87	0.86
PXSFS	0.41	0.56	0.37
SPXSFS	0.30	0.41	0.25

TABLE II. Summation of absorption reaction rate errors of case 1

Method	Absorption error/%	RMS/%	AVE/%
CSM	0.33	2.84	1.45
SLAS	-0.07	2.69	1.26
NDAS	0.59	1.81	1.14
CM	0.87	0.89	0.88
PXSFS	0.34	0.31	0.26
SPXSFS	0.35	0.31	0.28

TABLE III. Summation of absorption reaction rate errors of case 2

ACKNOWLEDGMENTS

This work is supported by the National Natural Science Foundation of China 11522544 and 11605128, China Postdoctoral Science Foundation funded project 2015M580854 and China Schorlarship Council.

REFERENCES

1. A. HÉBERT, "The ribon extended self-shielding model," *Nuclear science and engineering*, **151**, 1–24 (2005).
2. A. HÉBERT, *Applied reactor physics*, Presses inter Polytechnique (2009).
3. A. HÉBERT, "Development of the subgroup projection method for resonance self-shielding calculations," *Nuclear Science and Engineering*, **162**, 56–75 (2009).
4. T. TAKEDA and Y. KANAYAMA, "A Multiband Method with Resonance Interference Effect," *Nuclear Science and Engineering*, **131**, 401–410 (1999).
5. H. G. JOO, B. S. HAN, C. H. KIM, and K.-S. KIM, "Implementation of Subgroup Method In Direct Whole Core Transport Calculation Involving Nonuniform Temperature Distribution," in "Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications," (2005).
6. Y. S. JUNG, C. H. LIM, and H. G. JOO, "Temperature dependent subgroup formulation with number density adjustment for direct whole core power reactor calculation," *Annals of Nuclear Energy*, **96**, 249–263 (2016).
7. H. MATSUMOTO, M. OUISLOUMEN, and T. TAKEDA, "Spatially Dependent Self-Shielding Method with Temperature Distribution for the Two-Dimensional Transport Code PARAGON," *Journal of Nuclear Science and Technology*, **43**, *11*, 1311–1319 (2006).